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A Highly Accurate and Optimal Method to Calculate Long Range Interactions

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1 Systems with Long-Ranged Interactions

Generally, interactions between particles may be classified into short- and long-range interactions. Potentials, which are long-ranged exhibit a functional dependence with a decay slower than $1/r^d$, where d is the dimension of the physical space. Examples for this type of potential are the electrostatic or the gravitational potentials.

Considering long range interactions in atomistic simulations without simplifying assumptions, is a computationally very demanding task. Since all particle-particle interactions are of importance, no cut-off radius can be introduced, beyond which interactions are artificially set to zero. Therefore, a straight forward implementation of long range interaction potentials results in a computational complexity of $\mathcal{O}(N^2)$, if N is the number of particles. More advanced algorithms have been developed for periodic or open system geometries, which scale like $\mathcal{O}(N \log N)$ (e.g. P3M[3] for periodic systems), or $\mathcal{O}(N)$ (e.g. FMM[1] for open systems).

In the present article a fast and accurate procedure of complexity $\mathcal{O}(N)$ is described, which is based on a multigrid technique.

2 Particle-Mesh Methods

In order to calculate the electrostatic energy of particle i, the sum

$$U_i = \frac{1}{4\pi} \sum_{j=1, j\neq i}^{N} q_i q_j \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}$$

has to be evaluated, where $|\cdot|$ is the Euclidean distance and $\mathbf{x}_k$ and q_k denote the position and the charge of particle k.

Instead of doing so, the potential due to all charges except for charge i may also be calculated using Poisson's equation

$$\Delta\Phi(\mathbf{x}) = f(\mathbf{x}) = \sum_{j=1, j\neq i}^{N} q_j \delta(\mathbf{x} - \mathbf{x}_j). \tag{1}$$

In this case, the electrostatic energy of particle i is readily calculated as

$$U_i = q_i \Phi(\mathbf{x}_i).$$

To calculate the energies for all particles, N Poisson equations would have to be solved. Therefore, in order to reduce the computational time, the right hand side of Eq. 1 is modified so that all particles in the system are included at the same time. Solving this equation yields a potential energy surface to which all particles contribute. In order to calculate energies for single particles, the self-energy contribution has to be corrected. Usually, equations of type Eq. 1 are solved using finite difference shemes, i.e. the PDE is discretized on a uniform grid and the charges are assigned to the mesh using an appropriate scheme like nearest-grid-point (NGP) or cloud-in-cell (CIC)[3]. The linear system can then be solved using standard methods, e.g. Particle-Mesh (PM) method, as described by Hockney and Eastwood[3].

PM works well for fine grids which separate the particles from each other. In order to work with coarser grids which contain particles in neighboring or even the same boxes, a splitting similar to the splitting used in the Ewald summation can be used. The potential is splitted using the identity

$$\frac{1}{r} = \frac{f(r)}{r} + \frac{1 - f(r)}{r}$$

where a possible choice is $1 - f(r) = \mathrm{erf(r)}$, which corresponds to the potential of a Gaussian charge distribution. The Particle-Particle-Particle-Mesh method developed by Hockney and Eastwood[3] uses charge assignments to the mesh (with e.g. CIC), splitting of the potential into near- and far-field and the appropriate near-field correction to calculate the forces and energies due to the slow-decaying Coulomb-potential. If working in periodic systems, an efficient method to solve the linear system is based on a Fourier-transform technique where the fast Fourier transform can be applied, which results in a computational complexity of $\mathcal{O}(N \log N)$.

3 Multigrid Methods

Multigrid methods are known to be optimal solvers for linear systems arising from the discretization of elliptic PDEs. An introduction can be found for example in the books of Hackbusch[2] or Trottenberg et al.[6]. The idea of multgrid methods is quite simple: If a linear system is solved using an iterative solver like Jacobi or Gauß-Seidel, the iteration converges rather slowly, but the high frequency components of the error are smoothed very fast. To speed up the solution process, the system is being solved on a hierarchy of grids, so that each frequency component is treated on the appropriate grid.

In order to achieve an optimal scaling (i.e. $\mathcal{O}(N)$), in the present work a multigrid method is applied to solve Poisson's equation. A Gauß-Seidel relaxation scheme is used in combination with a forth order dicretization of the Laplace operator[5]. In case of systems with open boundaries, Dirichlet conditions are imposed on the surface of the (finite) computational domain. For a fast evaluation of boundary potentials a multipole expansion with computational complexity $\mathcal{O}(N)$ is used as described in the paper of Sutmann and Steffen[4].

4 B-Spline Densities

Since a multigrid method is used to solve the PDE, there is no need to work in Fourier space. Therefore the use of an FFT can be avoided completely. As a splitting scheme to

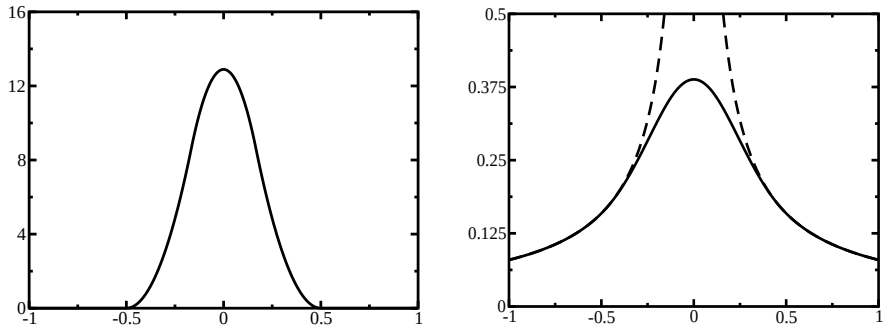

Figure 1. Left: radial shape of a charged centered, quadratic and normalized B-spline density. Right: potential of a B-spline density. The potential of a point charge, exhibiting a divergence at $r = 0$, is shown for comparison.

seperate near and far field contributions a density with finite support is used. Instead of using the conventional choice $1 - f(r) = \mathrm{erf(r)}$ the present work makes use of a form for $1 - f(r)$ which corresponds to the potential of a uniformly charged B-spline density.

Considering the centered, quadratic and normalized B-spline with width $2R$ given by

$$\rho_B(\mathbf{x}) = \begin{cases} \dfrac{-486|\mathbf{x}|^2 + 162R^2}{32\pi R^5} & : \quad |\mathbf{x}| < \frac{R}{3} \\ \dfrac{486|\mathbf{x}|^2 - 972|\mathbf{x}|R + 486R^2}{64\pi R^5} & : \quad \frac{R}{3} \leq |\mathbf{x}| \leq R \\ 0 & : \quad R < |\mathbf{x}| \end{cases},$$

the corresponding potential is calculated via

$$\Phi_B(\mathbf{x}) = \frac{1}{4\pi} \int\limits_{\mathbb{R}^3} \frac{\rho_B(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}\, d\mathbf{x}'$$

and can be given in analytical form as

$$\Phi_B(\mathbf{x}) = \begin{cases} \dfrac{3(81|\mathbf{x}|^4 - 90|\mathbf{x}|^2R^2 + 65R^4)}{4\pi 80R^5} & : \quad |\mathbf{x}| < \frac{R}{3} \\ \dfrac{-243|\mathbf{x}|^5 + 810|\mathbf{x}|^4R - 810|\mathbf{x}|^3R^2 + 405|\mathbf{x}|R^4 - 2R^5}{4\pi|\mathbf{x}|160R^5} & : \quad \frac{R}{3} \leq |\mathbf{x}| \leq R \\ \dfrac{1}{4\pi|\mathbf{x}|} & : \quad R < |\mathbf{x}| \end{cases}$$

The B-spline densities are centered on the charges in the system and sampled onto the mesh in order to compute the right hand side of the PDE. The influence of this charge discretization to particles closer than distance R is taken into account by direct summing up the near-field contributions by explicit particle-particle calculations. Therefore, in this step the charge assignment to the grid and the associated error is avoided.

5 Conclusion

In the present work a mesh-based particle simulation method was presented which avoids the Fourier-space and the FFT completely using a multigrid technique to solve the Poisson equation. Overall the method results in an optimal computational complexity of $\mathcal{O}(N)$. First numerical experiments show very good accuracy. At the moment work is in progress to reliably estimate errors and to parallelize the method.

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